

Phenol, 3-methoxy-5-(2-phenylethyl)-  
17635-59-5 | DTXSID80170114

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.57

Global applicability domain: Inside

Local applicability domain index: 6.08e-01

Confidence level: 8.00e-01

Nearest Neighbors from the Training Set

Image not found

(4-cyclohexylphenoxy)acetic acid

Measured: 3.79

Predicted: 4.02

Image not found

Naproxen

Measured: 3.18

Predicted: 2.66

Image not found

4-(1-naphthyloxy)butanoic acid

Measured: 3.50

Predicted: 3.11